LECTURE 14

NUMERICAL INTEGRATION

- Find

$$I = \int_a^b f(x)dx$$

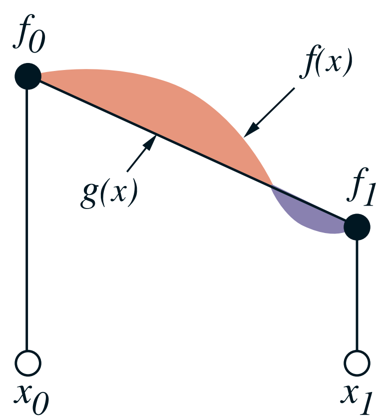
or

$$I = \int_a^b \left[\int_{u(x)}^{v(x)} f(x, y)dy \right] dx$$

- Often integration is required. However the form of $f(x)$ may be such that analytical integration would be very difficult or impossible. Use numerical integration techniques.
- Finite element (FE) methods are based on integrating errors over a domain. Typically we use numerical integrators.
- ***Numerical integration methods are developed by integrating interpolating polynomials.***

Trapezoidal Rule

- Trapezoidal rule uses a first degree Lagrange approximating polynomial ($N = 1$, $N+1 = 2$ nodes, linear interpolation).



- Define the linear interpolating function

$$g(x) = f_o\left(\frac{x_1 - x}{x_1 - x_o}\right) + f_1\left(\frac{x - x_o}{x_1 - x_o}\right)$$

- Establish the integration rule by computing $I = \int_{x_o}^{x_1} f(x)dx = \int_{x_o}^{x_1} (g(x) + e(x))dx$

$$I = \int_{x_o}^{x_1} g(x)dx + E \quad \Rightarrow$$

$$I = \int_{x_o}^{x_1} \left[f_o\left(\frac{x_1 - x}{x_1 - x_o}\right) + f_1\left(\frac{x - x_o}{x_1 - x_o}\right)\right]dx + E \quad \Rightarrow$$

$$I = \left[f_o\left(\frac{x_1 x - \frac{x^2}{2}}{x_1 - x_o}\right) + f_1\left(\frac{\frac{x^2}{2} - x_o x}{x_1 - x_o}\right)\right]_{x_o}^{x_1} + E \quad \Rightarrow$$

$$I = \left[f_o\left(\frac{x_1^2 - \frac{x_1^2}{2}}{x_1 - x_o}\right) + f_1\left(\frac{\frac{x_1^2}{2} - x_o x_1}{x_1 - x_o}\right) - f_o\left(\frac{x_1 x_o - \frac{x_o^2}{2}}{x_1 - x_o}\right) - f_1\left(\frac{\frac{x_o^2}{2} - x_o^2}{x_1 - x_o}\right) + E\right]$$

- **Trapezoidal Rule**

$$\boldsymbol{I = \left(\frac{x_1 - x_o}{2}\right)[f_o + f_1] + E}$$

- Trapezoidal Rule integrates the area of the trapezoid between the two data or interpolation points.

- Evaluating the error for trapezoidal rule.

  - The error E is dependent on the integral of the difference $e(x) = f(x) - g(x)$. However integrating the ξ dependent error approximation for the interpolating function does not work out in general since ξ is a function of x!

  - We must express $e(x)$ in terms of a series of terms expanded about x_o in order to evaluate $E = \int_{x_o}^{x_1} e(x)dx$ correctly.

  - An alternative strategy is to evaluate

$$E = \int_{x_o}^{x_1} f(x)dx - \left(\frac{x_1 - x_o}{2}\right)(f_o + f_1)$$

    by developing Taylor series expansions for $f(x)$, f_o and f_1.

  - We do note that as $x_1 - x_o = h \downarrow 0 \Rightarrow E \downarrow 0$

Evaluation of the Error for Trapezoidal Rule

Evaluation of the error by integrating e(x)

- We note that

$$E \equiv I - \int_{x_o}^{x_N} g(x)dx \quad \Rightarrow \quad E \equiv \int_{x_o}^{x_N} f(x)dx - \int_{x_o}^{x_N} g(x)dx$$

- However

$$e(x) \equiv f(x) - g(x) \quad \Rightarrow \quad \int_{x_o}^{x_N} e(x)dx = \int_{x_o}^{x_N} f(x)dx - \int_{x_o}^{x_N} g(x)dx$$

- Thus

$$E = \int_{x_o}^{x_N} e(x)dx$$

- Recall that $e(x)$ for Lagrange interpolation was expressed as:

$$e(x) = \frac{(x - x_o)(x - x_1)\dots(x - x_N)}{(N+1)!} f^{(N+1)}(\xi)$$

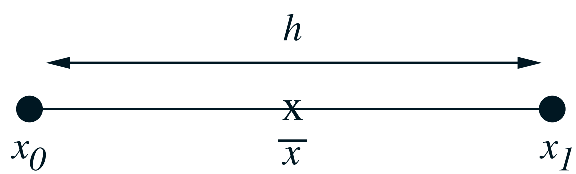
- Notes
  - Procedure applies to higher order integration rules as well.
  - In general ξ is a function of x
  - Neglecting the dependence of $\xi(x)$, can lead to incorrect results. e.g. for Simpson's $\frac{1}{3}$ rule you will integrate out the ξ dependent term and the result would be $E = 0$!
  - A way you can apply $E = \int_{x_o}^{x_1} e(x)dx$ is to take $e(x)$ as a series of terms! Then we will always get the correct answer!

<u>Evaluation of the error for Trapezoidal Rule by Taylor Series expansion</u>

$$E = I - \left(\frac{x_1 - x_o}{2}\right)[f_o + f_1] \qquad \Rightarrow$$

$$E = \int_{x_o}^{x_1} f(x)dx - \left(\frac{x_1 - x_o}{2}\right)(f_o + f_1)$$

- Let's now develop Taylor series expansions for $f(x)$, f_o and f_1 about $\bar{x} = \dfrac{x_o + x_1}{2}$



- In general Taylor series expansion about $\bar{x}$:

$$f(x) = f(\bar{x}) + (x-\bar{x})f^{(1)}(\bar{x}) + \frac{(x-\bar{x})^2}{2!}f^{(2)}(\bar{x}) + O(x-\bar{x})^3$$

- Now evaluate $f_o = f(x_o)$ using the Taylor series

$$f_o = f(\bar{x}) + (x_o-\bar{x})f^{(1)}(\bar{x}) + \frac{(x_o-\bar{x})^2}{2}f^{(2)}(\bar{x}) + O(x_o-\bar{x})^3$$

  - However since $x_o - \bar{x} = -\dfrac{h}{2}$

$$f_o = f(\bar{x}) - \frac{h}{2}f^{(1)}(\bar{x}) + \frac{h^2}{8}f^{(2)}(\bar{x}) + O(h)^3$$

- Similarly

$$f_1 = f(\bar{x}) + \frac{h}{2} f^{(1)}(\bar{x}) + \frac{h^2}{8} f^{(2)}(\bar{x}) + O(h)^3$$

- Let's substitute in for $f(x)$, f_o and f_1 into the expression for E

$$E = \int_{x_o}^{x_1} \left[f(\bar{x}) + (x - \bar{x}) f^{(1)}(\bar{x}) + \frac{(x-\bar{x})^2}{2!} f^{(2)}(\bar{x}) + O(x-\bar{x})^3 \right] dx$$

$$-\left(\frac{x_1 - x_0}{2}\right)\left[f(\bar{x}) - \frac{h}{2} f^{(1)}(\bar{x}) + \frac{h^2}{8} f^{(2)}(\bar{x}) + O(h)^3 + f(\bar{x}) + \frac{h}{2} f^{(1)}(\bar{x}) + \frac{h^2}{8} f^{(2)}(\bar{x}) + O(h)^3 \right]$$

$$\Rightarrow$$

$$E = \left[f(\bar{x}) x + \frac{(x-\bar{x})^2}{2} f^{(1)}(\bar{x}) + \frac{(x-\bar{x})^3}{6} f^{(2)}(\bar{x}) + O(x-\bar{x})^4 \right]_{x_o}^{x_1}$$

$$- \frac{(x_1 - x_o)}{2}\left[2f(\bar{x}) + \frac{h^2}{4} f^{(2)}(\bar{x}) + O(h)^3 \right]$$

$$\Rightarrow$$

$$E = f(\bar{x})(x_1 - x_o) + \frac{(x_1 - \bar{x})^2}{2} f^{(1)}(\bar{x}) - \frac{(x_o - \bar{x})^2}{2} f^{(1)}(\bar{x})$$

$$+ \frac{(x_1 - \bar{x})^3}{6} f^{(2)}(\bar{x}) - \frac{(x_o - \bar{x})^3}{6} f^{(2)}(\bar{x}) + O(x_1 - \bar{x})^4 + O(x_o - \bar{x})^4$$

$$-(x_1 - x_o) f(\bar{x}) - \frac{(x_1 - x_o)}{8} h^2 f^{(2)}(\bar{x}) + \frac{(x_1 - x_o)}{2} O(h)^3$$

$$\Rightarrow$$

$$E = \frac{h^2}{8} f^{(1)}(\bar{x}) - \frac{h^2}{8} f^{(1)}(\bar{x}) + \frac{h^3}{48} f^{(2)}(\bar{x}) + \frac{h^3}{48} f^{(2)}(\bar{x}) + O(h)^4 - \frac{h^3}{8} f^{(2)}(\bar{x}) + O(h)^4$$

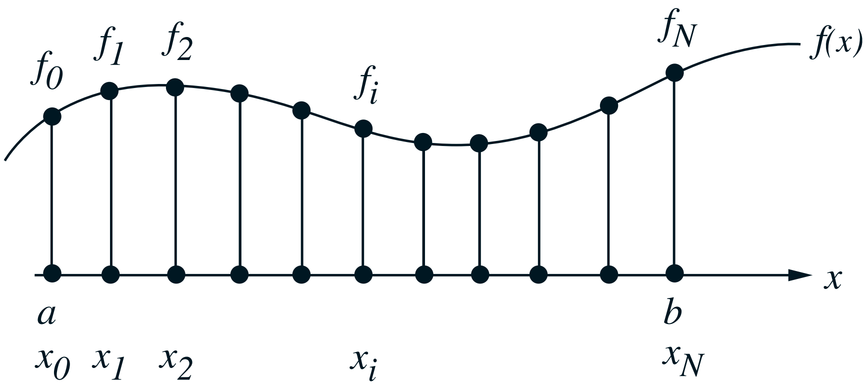
$$\Rightarrow$$

$$\mathbf{E = -\frac{h^3}{12} f^{(2)}(\bar{x})}$$

- Notes
  - Higher order terms have been truncated in this error expression.
  - This integration will be exact only for $f(x) =$ linear.
  - However it is *third* order accurate in h
  - Error evaluation procedure using T.S. applies to higher order methods as well

Extended Trapezoidal Rule

- Apply trapezoidal rule to multiple *"sub-intervals"*



- Integrate each sub-interval with trapezoidal rule and sum
  - Split $[a, b]$ into N equispaced sub-intervals with $h = \frac{b-a}{N}$
  - Compute I as:

$$I = \int_a^b f(x)dx = \sum_{i=0}^{N-1} \left(\int_{x_i}^{x_{i+1}} f(x)dx \right) \quad \Rightarrow$$

$$I = \left(\frac{x_1 - x_o}{2}\right)(f_o + f_1) + \left(\frac{x_2 - x_1}{2}\right)(f_1 + f_2) + \ldots + \left(\frac{x_N - x_{N-1}}{2}\right)(f_{N-1} + f_N) + E_{[a,b]}$$

$$\Rightarrow$$

$$I = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{N-1} + f_N) + E_{[a,b]}$$

where

$$f_o = f(a)$$

$$f_1 = f(a+h)$$

$$f_2 = f(a+2h)$$

$$\vdots$$

$$f_i = f(a+ih)$$

- Thus extended trapezoidal rule can be expressed as:

$$\boldsymbol{I = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{N-1} f(a+ih)\right] \quad \text{where} \quad N = \frac{b-a}{h}}$$

- Error is simply the sum of the individual errors:

$$E_{[a,b]} = \sum_{i=1}^{N} -\frac{1}{12}h^3 f^{(2)}(\bar{x}_i)$$

where $\bar{x}_i$ = the average x within each sub-interval

$$E_{[a,b]} = -\frac{1}{12}(b-a)h^2 \cdot \frac{1}{N}\sum_{i=1}^{N} f^{(2)}(\bar{x}_i)$$

- Defining the average of the second derivatives

$$\overline{f^{(2)}} \equiv \frac{1}{N}\sum_{i=1}^{N} f^{(2)}(\bar{x}_i)$$

- Thus

$$\boldsymbol{E_{[a,b]} = -\frac{1}{12}(b-a)h^2\overline{f^{(2)}}}$$

- Error is 2nd order over the interval $[a, b]$
  - Thus the error over the interval decreases as h^2.
  - The slope of error vs. h on a log-log plot is 2.

Romberg Integration

- Uses extended trapezoidal rule with two or more different integration point to integration point spacings (in this case equal to the sub-interval spacing), h, in ***conjunction*** with the general form of the error in order to compute one or more terms in the series which represents the error.
  - This will then result in a higher order estimate of the integrand.
  - More importantly, it will allow us to easily derive an error estimate for the numerical integrations based on the results using the different grid spacings.
- Consider

$$I = \tilde{I}_h + E_{[a,b]-h}$$

where

$I \equiv$ the exact integrand,

$\tilde{I}_h \equiv$ the approximate integral with integration point to integration point spacing h

$E_{[a,b]-h} \equiv$ the associated error.

$$\tilde{I}_h \equiv \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{\left(\frac{b-a}{h}-1\right)} f(a+ih)\right]$$

- In general the form of the error term if we had worked out more terms in the error series.

$$E_{[a,\,b]-h} = Ch^2 + Dh^4 + Eh^6 + O(h)^8$$

- Notes

  - The coefficient $C = -\frac{1}{12}(b-a)\overline{f^{(2)}}$

  - In general, C, D, E etc. are functions of the average of the various derivatives of f over the interval of interest.

  - These coefficients are not dependent on the spacing h.

  - Also we do not worry about the exact form of these coefficients.

  - As far as we are concerned, they are unknown constant coefficients over the interval $[a, b]$.

- **Thus the integral**

$$I = \tilde{I}_h + Ch^2 + Dh^4 + Eh^6 + O(h)^8$$

  - **Unknowns: I = the exact integral; $C, D, E \ldots$ = the coefficients of the error term.**
  - **Knowns: $\tilde{I}_h$ = the approximation to the integral; h = the integration point spacing.**

- We must generate equations to solve for some of the unknowns
  - Solve for I and C. This will improve the accuracy of I to $O(h)^4$!

- Two unknowns ⇒ must have two equations ⇒ use two different integration point to integration point spacings.

$$I = \tilde{I}_{h_1} + Ch_1^2 + Dh_1^4 + Eh_1^6 + O(h_1)^8$$

$$I = \tilde{I}_{h_2} + Ch_2^2 + Dh_2^4 + Eh_2^6 + O(h_2)^8$$

- We now have two equations and can therefore solve for 2 unknowns.
  - I = the exact integral is unknown: C = the leading coefficient of the error term is unknown.
  - We can solve for I and C.
  - We can not solve for D, E, ... and the other coefficients since we do not have enough equations!
- We must select h_1 and h_2 such that $[a, b]$ is divided into an integer number of sub-intervals. Let

$$h_1 = 2h_*$$

$$h_2 = h_* = base\ interval$$

- We compute the approximation to the integral twice.

$$2h_* \rightarrow \tilde{I}_{2h_*}$$

$$h_* \rightarrow \tilde{I}_{h_*}$$

- Thus

$$I = \tilde{I}_{2h_*} + 4Ch_*^2 + 16Dh_*^4 + 64Eh_*^6 + O(h_*)^8$$

$$I = \tilde{I}_{h_*} + Ch_*^2 + Dh_*^4 + Eh_*^6 + O(h_*)^8$$

- Two equations and 2 unknowns. Thus we can solve for both I and C.

$$-I = -\tilde{I}_{2h_*} - 4Ch_*^2 - 16Dh_*^4 - 64Eh_*^6 + O(h_*)^8$$

$$4I = 4\tilde{I}_{h_*} + 4Ch_*^2 + 4Dh_*^4 + 4Eh_*^6 + O(h_*)^8$$

$$\Rightarrow$$

$$\mathbf{I = \frac{4\tilde{I}_{h_*} - \tilde{I}_{2h_*}}{3} - 4Dh_*^4 - 20Eh_*^6 + O(h_*)^8}$$

- Therefore if you have 2 second order accurate approximations to I

$\tilde{I}_{h_*}$ using h_*

$\tilde{I}_{2h_*}$ using $2h_*$

You can extrapolate a 4th order accurate approximation using the above formula.

- More importantly, we can estimate the errors for both the coarse and the fine integration point solutions simply by solving for C using the 2 simultaneous equations

$$C = \frac{\tilde{I}_{h_*} - \tilde{I}_{2h_*}}{3h_*^2} - 5Dh_*^2 + O(h_*)^4$$

- Thus the estimated error associated with the ***coarse*** integration point spacing solution, using the coarse $2h_*$ and fine h_* integration point spacing solutions is,

$$E_{[a,b]-2h_*} = \frac{4}{3}(\tilde{I}_{h_*} - \tilde{I}_{2h_*}) + O(h_*)^4$$

- The estimated error associated with the ***fine*** integration point spacing solution, using the coarse $2h_*$ and fine h_* integration point spacing solutions is,

$$E_{[a,b]-h_*} = \frac{1}{3}(\tilde{I}_{h_*} - \tilde{I}_{2h_*}) + O(h_*)^4$$

Example

- Consider:

$$I = \int_0^8 \left(\frac{5x^4}{8} - 4x^3 + 2x + 1\right) dx$$

- Integrating exactly $I = 72$

- Let's integrate numerically

$$f(x) = \frac{5x^4}{8} - 4x^3 + 2x + 1 \qquad a = 0 \qquad b = 8$$

- Apply extended trapezoidal rule using:
    - $h = 2h_* = 8$ (using one interval of 8)
    - $h = h_* = 4$ (using two intervals of 4)

- Apply the Romberg integration rule we derived when two integral estimates were obtained using intervals $2h_*$ and h_* to obtain a fourth order estimate for the integral

- Estimate the errors associated with the extended trapezoidal rule results

- Applying $h = 2h_* = 8$ (using one interval of 8)

$$\tilde{I}_{2h_*} = \frac{2h_*}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{\left(\frac{8-0}{2h_*}-1\right)} f(0 + i2h_*)\right] \Rightarrow$$

$$\tilde{I}_{2h_*} = 4\left[f(0) + f(8) + 2\sum_{i=1}^{0} f(0 + i2h_*)\right]$$

- Since the index i runs from 1 to 0, we do not evaluate the summation term. Thus

$$\tilde{I}_{2h_*} = 4[1 + 529] \Rightarrow$$

$$\tilde{I}_{2h_*} = 2120$$

- Applying $h = h_* = 4$ (using two intervals of 4)

$$\tilde{I}_{h_*} = \frac{h_*}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{\left(\frac{8-0}{h_*}-1\right)} f(a+ih)\right] \Rightarrow$$

$$\tilde{I}_{h_*} = 2\left[f(0) + f(8) + 2\sum_{i=1}^{1} f(0+4i)\right] \Rightarrow$$

$$\tilde{I}_{h_*} = 2[f(0) + f(8) + 2f(4)] \Rightarrow$$

$$\tilde{I}_{h_*} = 2[1 + 529 + 2 \times 87] \Rightarrow$$

$$\tilde{I}_{h_*} = 712$$

- We can obtain an $O(h_*)^4$ accurate answer using the $O(h_*)^2$ trapezoidal rule results, $\tilde{I}_{2h_*}$ and $\tilde{I}_{h_*}$

$$I = \frac{4\tilde{I}_{h_*} - \tilde{I}_{2h_*}}{3} + O(h_*)^4 \quad \Rightarrow$$

$$I = \frac{4 \times 712 - 2120}{3} + O(h_*)^4 \quad \Rightarrow$$

$$\mathbf{I = 242.6667 + O(h_*)^4}$$

- We can also estimate the error associated with the two $O(h_*)^2$ trapezoidal rule results, $\tilde{I}_{2h_*}$ and $\tilde{I}_{h_*}$
  - Let's estimate the error for the trapezoidal rule result with $h = 2h_* = 8$

$$E_{[a,b]-2h_*-estimated} = \frac{4}{3}(\tilde{I}_{h_*} - \tilde{I}_{2h_*}) + O(h_*)^4 = \frac{4}{3}(712 - 2120) = -1877.33$$

  - Note that the actual error for the trapezoidal rule results with $h = 2h_* = 8$

$$E_{[a,b]-2h_*-actual} = I - \tilde{I}_{2h_*} = 72 - 2120 = -2048.$$

- Let's estimate the error for the trapezoidal rule results with $h = h_* = 4$

$$E_{[a,b]-h_*-estimated} = \frac{1}{3}(\tilde{I}_{h_*} - \tilde{I}_{2h_*}) + O(h_*)^4 = \frac{1}{3}(712 - 2120) = -469.33$$

- Note that the actual error for the trapezoidal rule results with $h = h_* = 4$ equals

$$E_{[a,b]-h_*-actual} = I - \tilde{I}_{h_*} = 72 - 712 = -640.$$

Romberg Integration Using 3 Estimates of the Integral

- Let's consider using ***three*** estimates on I

$$I = \tilde{I}_{h_1} + Ch_1^2 + Dh_1^4 + Eh_1^6 + O(h_1)^8$$

$$I = \tilde{I}_{h_2} + Ch_2^2 + Dh_2^4 + Eh_2^6 + O(h_2)^8$$

$$I = \tilde{I}_{h_3} + Ch_3^2 + Dh_3^4 + Eh_3^6 + O(h_3)^8$$

- Three equations ⇒ we can solve for ***three*** unknowns: Solve for I = exact integral and C and D = ***coefficients*** of the first two terms in the error series!

- Therefore we can now derive an $O(h)^6$ accurate approximation to I

- Apply integration point spacings: $h_1 = 2h_*$, $h_2 = h_*$ and $h_3 = \frac{h_*}{2}$.

- Estimates of the integral are related to the exact integral, I, as:

$$I = \tilde{I}_{2h_*} + 4Ch_*^2 + 16Dh_*^4 + 64Eh_*^6 + O(h_*)^8$$

$$I = \tilde{I}_{h_*} + Ch_*^2 + Dh_*^4 + Eh_*^6 + O(h_*)^8$$

$$I = \tilde{I}_{\frac{h_*}{2}} + \frac{C}{4}h_*^2 + \frac{D}{16}h_*^4 + \frac{E}{64}h_*^6 + O(h_*)^8$$

- We can solve for the unknowns I, C and D!

$$I = \frac{1}{45}\left[64\tilde{I}_{\frac{h_*}{2}} - 20\tilde{I}_{h_*} + \tilde{I}_{2h_*}\right] + E(h_*)^6 + O(h_*)^8$$

SUMMARY OF LECTURE 14

- Trapezoidal rule is simply applying linear interpolation between two points and integrating the approximating polynomial.

- Error for Trapezoidal Rule

  - The error can be determined by computing $\int_{x_o}^{x_1} e(x)dx$ if $e(x)$ is expressed in series form.
  - The error can also be determined by Taylor series expansions of the integration formula and the exact integral.

- Extended trapezoidal rule applies piecewise linear approximations and sums up individual integrals.

- Error for extended trapezoidal rule is obtained simply by adding errors over all subintervals

- Romberg Integration
  - Uses trapezoidal rule with different intervals.
  - Extrapolates a better answer by estimating the error.
  - This can be a much more efficient process than increasing the number of intervals.
- Romberg Integration can be applied to any of the integration methods we will develop